Open Journal of
Discrete Applied Mathematics

PSR Press

Article

Some basic properties of Sombor indices

Ivan Gutman

Faculty of Science, University of Kragujevac, Kragujevac, Serbia.; gutman@kg.ac.rs

Communicated by: Muhammad Kamran Jamil
Received: 16 December 2020; Accepted: 2 January 2021; Published: 9 January 2021

Abstract: The recently introduced class of vertex–degree–based molecular structure descriptors, called Sombor indices (SO), are examined and a few of their basic properties established. Simple lower and upper bounds for SO are determined. It is shown that any vertex–degree–based descriptor can be viewed as a special case of a Sombor–type index.

Keywords: Molecular graph, topological index, degree (of vertex), metric space, degree-space, Sombor index.

MSC: 05C07, 05C09.

1. Introduction

In contemporary mathematical chemistry more than 30 various vertex–degree–based (VDB) molecular structure descriptors (topological indices) have been put forward. Both their physicochemical applicability and mathematical properties were extensively studied; for details see [1–5] and the references cited therein.

The general form of a VDB topological index is

$$TI = TI(G) = \sum_{ij} F(d_i, d_j), \tag{1}$$

where d_i is the degree (= number of first neighbors) of the i-the vertex, and the summation goes over all pairs of adjacent vertices of the underlying molecular graph G. $F(x, y)$ is an appropriately selected function with the property $F(x, y) = F(y, x)$.

To each VDB index based on the function $F(x, y)$, it is possible to associate a "reduced" index, replacing x and y by $x - 1$ and $y - 1$.

In the standard formulation of the theory of VDB topological indices, $TI(G)$ depends on the vertices of the graph G, so that to each vertex a single parameter is associated – namely the vertex degree.

In a recent paper [6], an alternative interpretation of VDB indices has been offered. According to [6], $TI(G)$ is viewed as depending on the edges of the graph G, so that to each edge a pair of parameters are associated – namely the degrees of the two end-points of the considered edge.

At the first glance, this new interpretation is precisely the same as the traditional one. However, there is a subtle difference.

Let ij denote the edge connecting the i-th and the j-th vertex of the considered graph G. Let $x = d_i$ and $y = d_j$ be the respective vertex degrees, and assume that $x \geq y$. Then an ordered pair (x, y) represents the edge ij.

The pair (x, y) can now be interpreted as a *point in a two-dimensional metric space* $\mathcal{D}_2$ [6]. In [6], Euclidean metric has been employed, as the simplest choice. Then, in particular, the distance of the point (x, y) from the origin is $\sqrt{x^2 + y^2}$. However, it is imaginable to use other distance function [7], but this is left as a task for the future.

The point $(y, x) \in \mathcal{D}_2$ is said to be the *dual* of the point $(x, y) \in \mathcal{D}_2$.

In what follows, we refer to (x, y) as to a *degree-point* of the *degree-space* $\mathcal{D}_2$. Then (y, x) is the *dual-degree-point*.

In the later considerations, a VDB topological index will play a distinguished role. This is the first Zagreb index, defined as

$$Zg = Zg(G) = \sum_i d_i^2 \,,$$

which happens to be historically the first VDB index, conceived as early as in the 1970s [9]. It is long time known [8] that Zg can be rewritten in the form (1) as

$$Zg = \sum_{ij} (d_i + d_j) \,. \tag{2}$$

The distance $r(x,y) = \sqrt{x^2+y^2}$ between the degree-point (x,y) and the origin $(0,0)$ is called the *degree-radius* of the edge ij [6]. By summing of $r(x,y)$ over all edges of the underlying graph G, and by bearing in mind Equation (1), we arrive at a new VDB structure descriptor, named *Sombor index* [6]:

$$SO = SO(G) = \sum_{ij} \sqrt{d_i^2 + d_j^2}, \tag{3}$$

and its reduced version

$$SO_{red} = SO_{red}(G) = \sum_{ij} \sqrt{(d_i-1)^2 + (d_j-1)^2} \,. \tag{4}$$

In the paper [6], several properties of the above defined Sombor indices have been determined. In what follows, we establish a few more.

2. Simple bounds for SO and SO_{red}

Theorem 1. *Let $Zg(G)$ be the first Zagreb index of the graph G and let G has m edges. Then*

$$Zg(G) < SO(G) \leq \frac{1}{\sqrt{2}}\, Zg(G), \tag{5}$$

and

$$Zg(G) - 2m < SO_{red}(G) \leq \frac{1}{\sqrt{2}}\, [Zg(G) - 2m]. \tag{6}$$

Equality on the right–hand side of (5) and (6) holds if and only if the graph G is regular or each of its components is regular.

Proof. Let $a \geq b \geq 1$ be real numbers. Then,

$$(a+b)^2 = a^2 + 2ab + b^2 > a^2 + b^2,$$

implying

$$a + b > \sqrt{a^2 + b^2} \,. \tag{7}$$

Bearing in mind Equations (2) and (3), we arrive at the left–hand side of (5).

From $(a-b)^2 \geq 0$, we get

$$a^2 + b^2 \geq 2ab \;\;\Leftrightarrow\;\; 2a^2 + 2b^2 \geq a^2 + b^2 + 2ab = (a+b)^2,$$

implying

$$\sqrt{2}\,\sqrt{a^2+b^2} \geq a + b \,. \tag{8}$$

Bearing in mind Equations (2) and (3), we arrive at the right–hand side of (5). Equality holds if $d_i = d_j$ for all edges of the graph G, i.e., if each component of G is a regular graph. If G is connected, then equality holds if and only if G is a regular graph.

The inequalities (6) are obtained by replacing in (7) and (8) a and b by $a-1$ and $b-1$, respectively. □

The bounds (5) and (6) have a far-reaching consequence: The Sombor index and its reduced form behave closely similar to the first Zagreb index Zg. A great variety of mathematical properties of Zg have been determined (for details see the survey [10]). Among these are numerous lower and upper bounds. These all could now be applied also to the Sombor and reduced Sombor indices.

In our opinion, the indices SO and SO_{red} are not of great applicability in QSPR and QSAR studies (since by Theorem 1, they only slightly differ from Zg). Their true value lies in their new interpretation, offering novel insights thanks to the use of the associated metric space.

3. Any VDB index is a Sombor-type index

In the paper [6], it was demonstrated that a particular VDB descriptor, namely the Albertson index is related to the distance between the degree-points and their duals. This means that the Albertson index, introduced a quarter-of-century ago [11], happens to be of Sombor-type. In [6], this concealed property of the Albertson index appeared to be a kind of surprise. It now becomes clear that this was no exception whatsoever.

We now show that any VDB index can be viewed as being of Sombor-type, i.e., as being related to the distance between the degree-points and some other elements of the degree-space.

In order to see this, to any degree-point (x, y) (pertaining to the edges of the corresponding graph G), we associate another degree point $(x+F, y+F) \in \mathcal{D}_2$, where F is the function specified in formula (1). Then the Euclidean distance between these two degree-points is

$$\sqrt{\big[(x+F)-x\big]^2 + \big[(y+F)-y\big]^2} = \sqrt{2}\,F,$$

which by summation over all edges of the graph G, and by taking into account Equation (1), becomes equal to $\sqrt{2}\,TI(G)$.

By the very same argument, we conclude that any reduced VDB index can be viewed as a reduced Sombor-type index.

Conflicts of Interest: "The author declares no conflict of interest."

References

[1] Dehmer, M., Varmuza, K., & Bonchev, D. (Eds.) (2012). *Statistical Modelling of Molecular Descriptors in QSAR/QSPR*. Weinheim: Wiley–Blackwell.

[2] Devillers, J., & Balaban, A. T. (Eds.) (1999). *Topological Indices and Related Descriptors in QSAR and QSPR*. Amsterdam: Gordon & Breach.

[3] Karelson, M. (2000). *Molecular Descriptors in QSAR/QSPR*. New York: Wiley.

[4] Kulli, V. R. (2020). Graph indices, in: Pal, M., Samanta, S., & Pal A. (Eds.), *Handbook of Research of Advanced Applications of Graph Theory in Modern Society*. Hershey: Global, pp. 66–91.

[5] Todeschini, R., & Consonni, V. (2009). *Molecular Descriptors for Chemoinformatics*. Wienheim: Wiley–VCH.

[6] Gutman, I. (2021). Geometric approach to degree–based topological indices: Sombor indices. *MATCH Communications in Mathematical and in Computer Chemistry, 86*, 11–16.

[7] Deza, M. M., & Deza, E. (2012). *Encyclopedia of Distances*. Heidelberg: Springer.

[8] Došlić, T., Furtula, B., Graovac, A., Gutman, I., Moradi, S., & Yarahmadi, Z. (2011). On vertex–degree–based molecular structure descriptors. *MATCH Communications in Mathematical and in Computer Chemistry, 66*, 613–626

[9] Gutman, I., & Trinajstić, N. (1972). Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons. *Chemical Physics Letters, 17*, 535–538.

[10] Borovićanin, B., Das, K. C., Furtula, B., & Gutman, I. (2017). Bounds for Zagreb indices. *MATCH Communications in Mathematical and in Computer Chemistry, 78*, 17–100.

[11] Albertson, M. O. (1997). The irregularity of a graph. *Ars Combinatoria, 46*, 219–225.